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The Equation of State of LLM-105 (2,6-diamino-3,5-dinitropyrazine-1-ox

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(2,6-diamino-3,5-dinitropyrazine-1-oxide)
San Antonio, TX, United States
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Lawrence Livermore National Laboratory

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March 4, 2015

APS March Meeting, San Antonio TX

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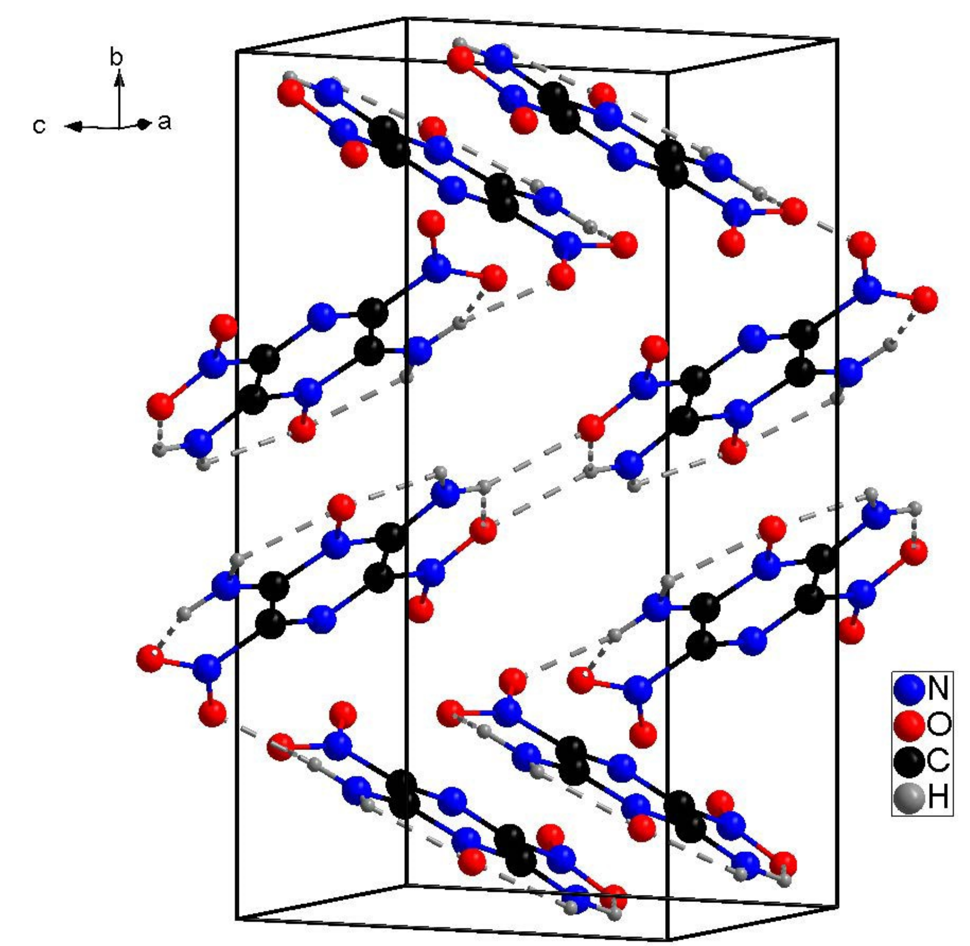
LLM-105 has a high density, detonation velocity, and is relatively difficult to initiate

Ambient Pressure Representation of LLM-105



Monoclinic structure (SG: P21/n (14))

Long-range H-bonding network

Theoretical results indicate phase transitions at 8, 17, 25, 42 GPa[1]

Theoretical results also indicate ambient phase stability to 45 GPa[2]

Previous Exp. work extends to 6 GPa[3]

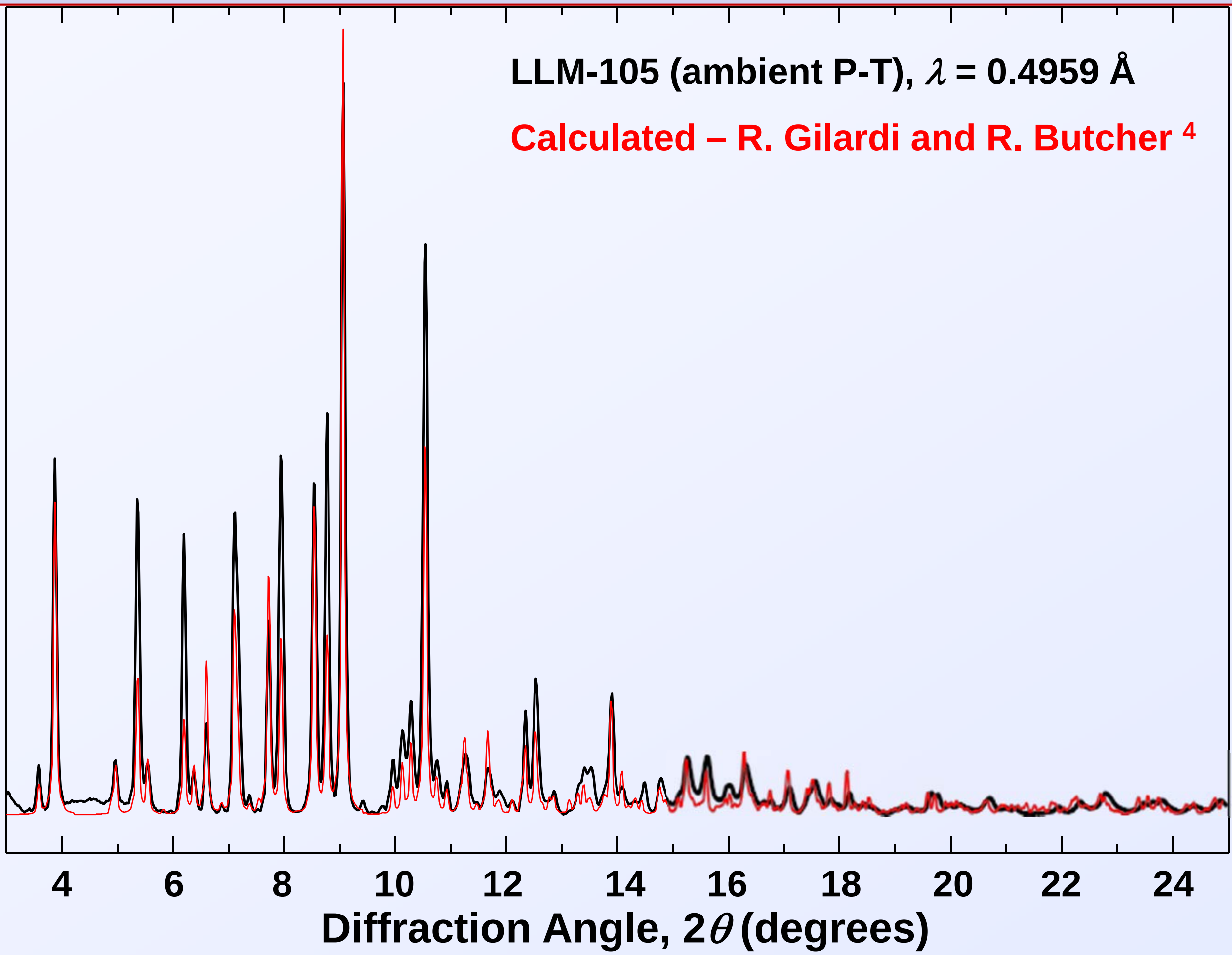
1. Q. Wu, C. Yang, Y. Pan, F. Xiang, Z. Liu, W. Zhu, and H. Xiao, *Journal of Molecular Modeling* 19, 5159 (2013).

2. M. R. Manaa, I.-F. W. Kuo, and L. E. Fried, *J. Chem. Phys.* 141, 064702 (2014).

3. J. C. Gump, C. A. Stoltz, B. P. Mason, B. G. Freedman, J. R. Ball, and S. M. Peiris, *J. Appl. Phys.* 110, 073523 (2011).

LLM-105 Powder Diffraction Bragg Peak Positions Match Well with Single Crystal X-ray Results

Ambient Pressure X-ray Powder Diffraction Pattern - LLM-105



Experimental Details

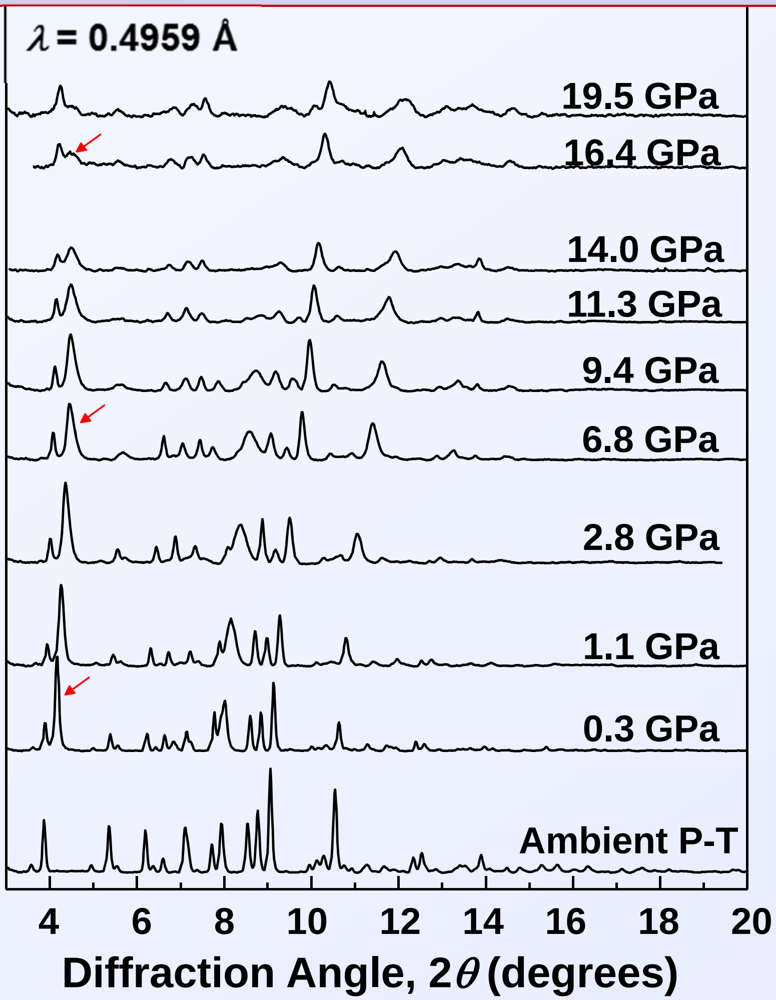
- Ground powder
- Silicone oil PTM
- Au & Ruby P sensors
- 400 μm diamond culets
- Re gasket

- XRD experiments LBNL/ALS on BL 12.2.2
- ~ 10 μm FW-HM spot
- 60s exposure per site
- FIT2D for integration
- GSAS LeBail Refinements

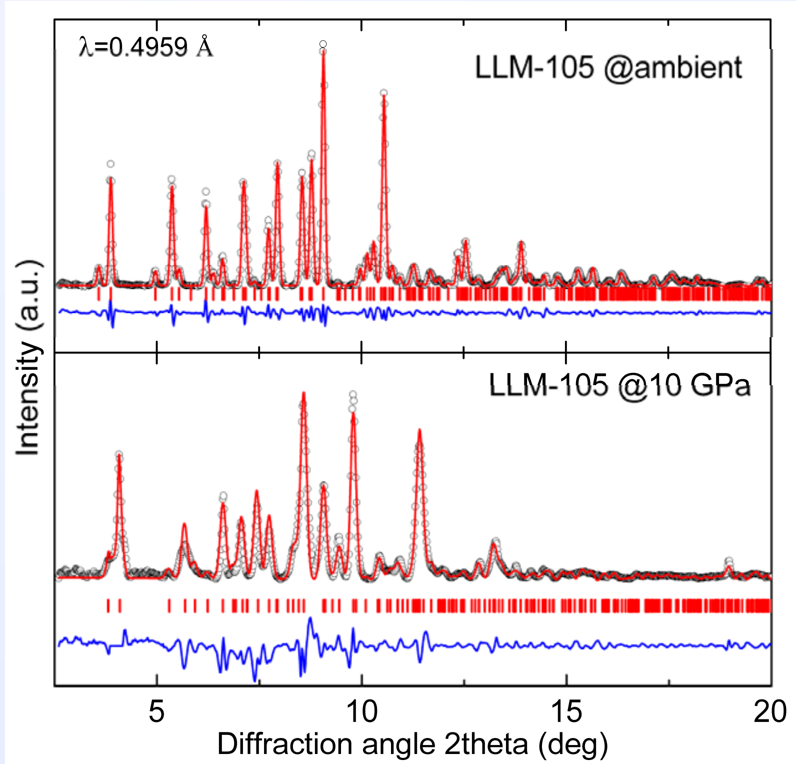
4. R. D. Gilardi and R. J. Butcher, *Acta Crystallographica Section E-structure Reports*, Online 57, o657 (2001).

Pressure Dependent Powder Diffraction Patterns Do Not Reveal a Structural Phase Transition

Pressure Dependent Diffraction Patterns



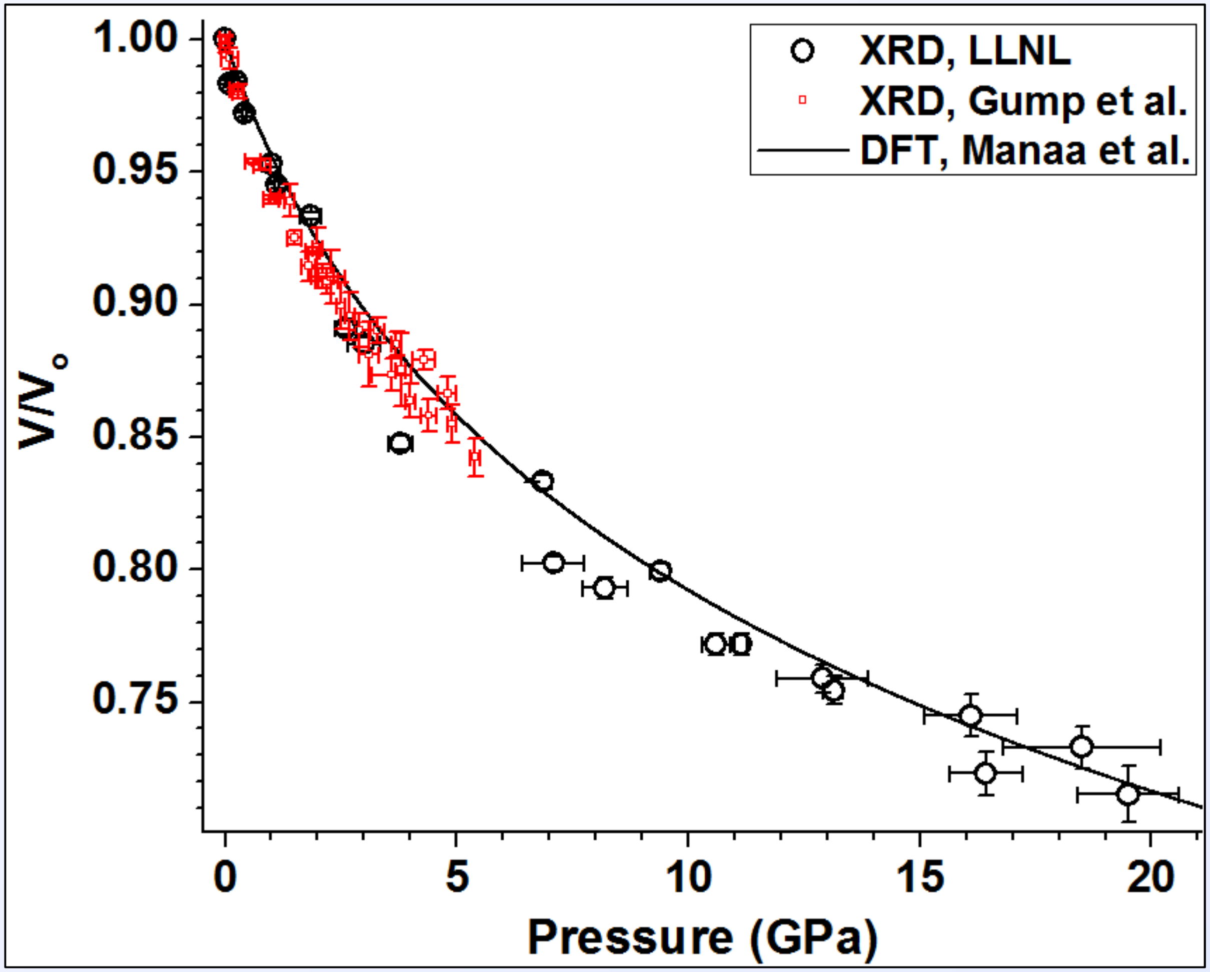
LeBail Powder Diffraction Refinements



With exception to one high d-spacing peak, (See: red arrow), all patterns index well to the monoclinic structure (SG: P21/n (14))

The Experimental LLM105 P-V EOS Matches Well to Recent Dispersion Corrected DFT Results

P-V EOS Comparison to Gump et al. and Manaa et al.



EOS Param. Comparisons

Weighted 3rd-order

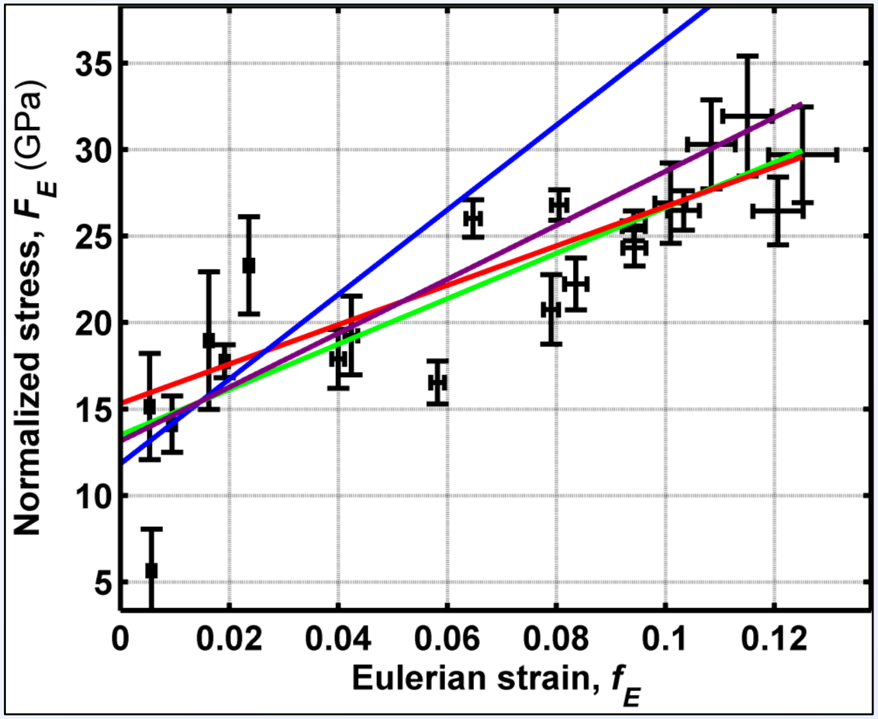
Birch-Murnaghan model

	LLNL XRD	DFT	Gump et al.
V_o (Å^3)	750.1	741.0	746.3
K_o (GPa)	11.8	19.7	10.2
K'_o	17.8	7.1	23.4

Single Crystal V_o = 748.2 Å^3

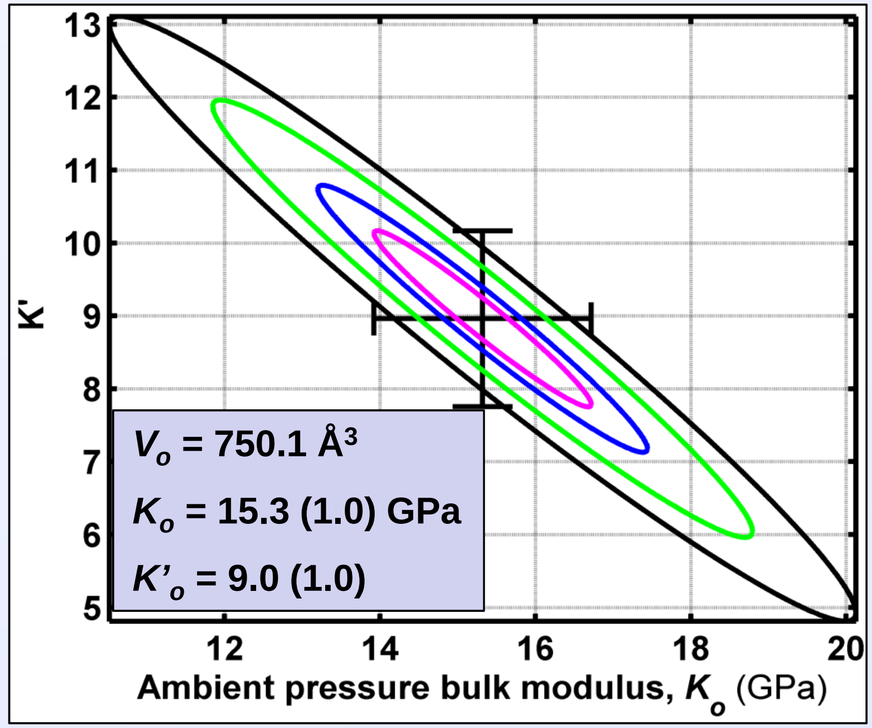
The EOS Model That Best Approximates our P-V EOS Data is the 1st-order *F-f* model

F-f EoS Model Fits



LLM105 cold-compression data fit to a first-order *F-f* model. The green line represents an unweighted fit and the red line is an experiment-ally weighted fit. The blue line is from a 3rd order B-M fit and the violet line is a Vinet EOS model fit.

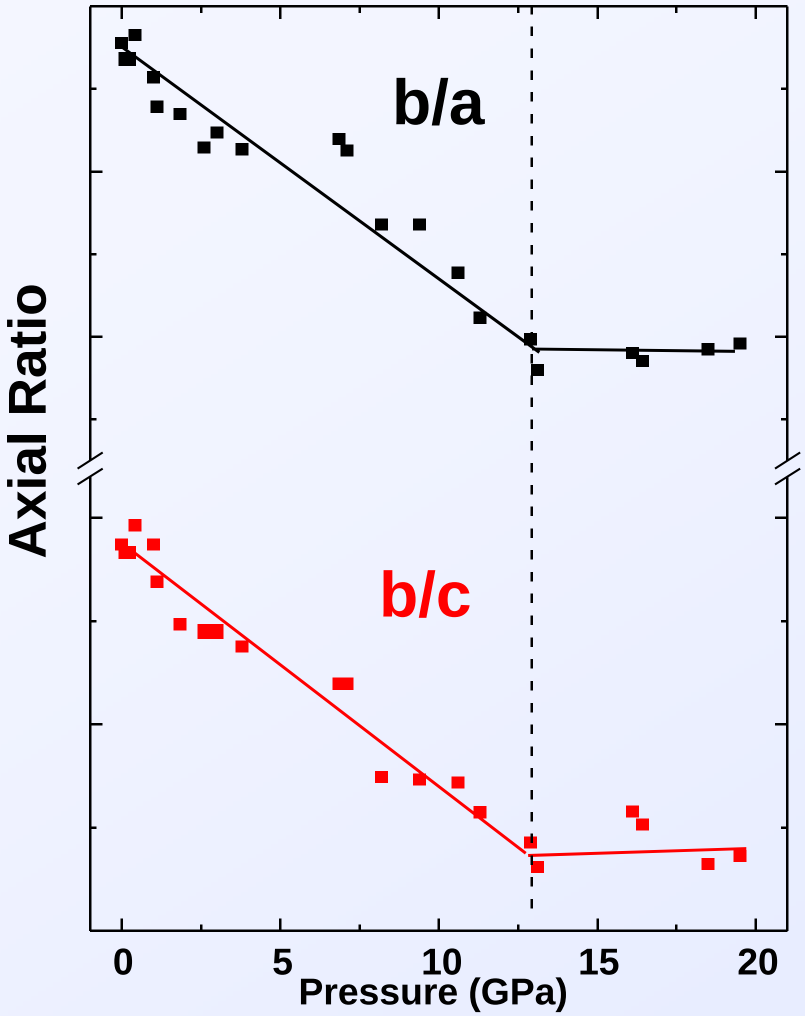
F-f 1st-order Confidence Ellipses



Confidence ellipses for the weighted *F-f* fit. The magenta colored ellipse is 0.607-σ, blue is 1-σ, green is 2-σ, and the black ellipse is 3-σ.

The Pressure Dependent Axial Ratios Reveal the Onset of Inter-Sheet Stiffening at ~ 13 GPa

Pressure dependent axial ratios



The b-axis is the most compressible

The change in slope at ~ 13 GPa signals a significant change in the relative compressibility along the b-axis (it matches the compressibility of the a and c axes)

At ~ 13 Gpa, the inter-sheet distance becomes nearly the same as intra-molecular distances

Questions?